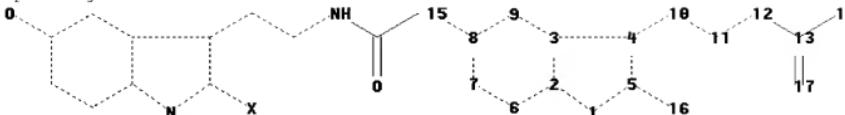


Structures uploaded into STN REGISTRY

Uploading L5.str



chain nodes :  
10 11 12 13 14 15 16 17

ring nodes :  
1 2 3 4 5 6 7 8 9

chain bonds :  
4-10 5-16 8-15 10-11 11-12 12-13 13-14 13-17

ring bonds :  
1-2 1-5 2-3 2-6 3-4 3-9 4-5 6-7 7-8 8-9

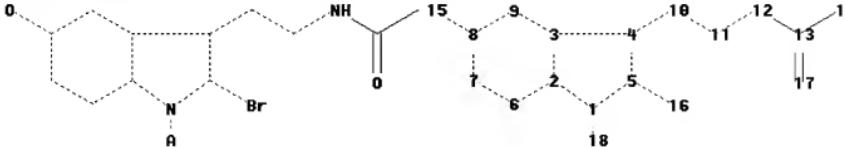
exact/norm bonds :  
1-2 1-5 2-3 2-6 3-4 3-9 4-5 4-10 5-16 6-7 7-8 8-9 8-15 10-11 11-12

12-13 13-17

exact bonds :  
13-14

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS

Uploading L29.str



chain nodes :  
10 11 12 13 14 15 16 17

ring nodes :  
1 2 3 4 5 6 7 8 9

ring/chain nodes :

18

chain bonds :  
1-18 4-10 5-16 8-15 10-11 11-12 12-13 13-14 13-17

ring bonds :  
1-2 1-5 2-3 2-6 3-4 3-9 4-5 6-7 7-8 8-9

exact/norm bonds :  
1-2 1-5 1-18 2-3 2-6 3-4 3-9 4-5 4-10 5-16 6-7 7-8 8-9 8-15 10-11

11-12 12-13 13-17

exact bonds :  
13-14

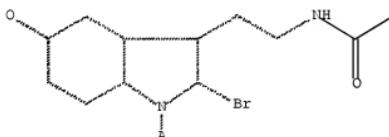
Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

Structure search history

=> d stat query L35  
L5 STR



Structure attributes must be viewed using STN Express query preparation.  
L7 66 SEA FILE=REGISTRY SSS FUL L5  
L29 STR



Structure attributes must be viewed using STN Express query preparation.  
L31 18 SEA FILE=REGISTRY SUB=L7 SSS FUL L29  
L32 7 SEA FILE=HCAPLUS SPE=ON ABB=ON PLU=ON L31  
L33 6 SEA FILE=HCAPLUS SPE=ON ABB=ON PLU=ON L32 AND (AY<2007 OR  
PY<2007 OR PRY<2007 OR REVIEW/DT)  
L34 6 SEA FILE=HCAPLUS SPE=ON ABB=ON PLU=ON L32 AND (THU/RL OR  
DGN/RL OR DMA/RL OR PAC/RL OR PKT/RL OR ADV/RL)  
L35 7 SEA FILE=HCAPLUS SPE=ON ABB=ON PLU=ON (L33 OR L34)

Structure search results

=> d L35 1-7 ibib ed abs hitrn hitstr

L35 ANSWER 1 OF 7 HCPLUS COPYRIGHT 2011 ACS on STN  
 ACCESSION NUMBER: 2010:175975 HCPLUS Full-text  
 DOCUMENT NUMBER: 152:231283  
 TITLE: Tryptophan derivatives for Osteoporosis therapy  
 INVENTOR(S): Somei, Masanori; Hattori, Atsuhi; Suzuki, Nobuo  
 PATENT ASSIGNEE(S): Japan  
 SOURCE: U.S., 13pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 7659304	B2	20100209	US 2008-7992	20080117 <--
US 20090054511	A1	20090226		
WO 2007010723	A1	20070125	WO 2006-JP312978	20060629 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRIORITY APPLN. INFO.: JP 2005-209753 A 20050720 <--  
                           WO 2006-JP312978 A2 20060629 <--

OTHER SOURCE(S): CASREACT 152:231283; MARPAT 152:231283

ED Entered STN: 11 Feb 2010

AB Tryptophan derivs. which can be used for treatment of osteoporosis and as an osteoblast activator is disclosed in this invention.

IT 920516-20-7P 920516-21-8P 920516-22-9P

920516-23-0P

RL: FAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)  
 (tryptophan derivs. for osteoporosis therapy)

IT 920516-24-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(tryptophan derivs. for osteoporosis therapy)

IT 920516-20-7P 920516-21-8P 920516-22-9P

920516-23-0P

RL: FAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)  
 (tryptophan derivs. for osteoporosis therapy)

IT 920516-20-7P 920516-21-8P 920516-22-9P

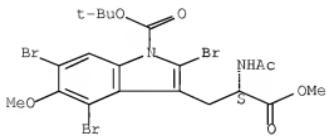
920516-23-0P

RL: FAC (Pharmacological activity); SPN (Synthetic preparation);  
 THU (Therapeutic use); BIOL (Biological study); PREP  
 (Preparation); USES (Uses)  
 (tryptophan derivs. for osteoporosis therapy)

RN 920516-20-7 HCPLUS

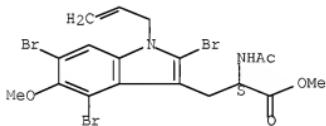
CN L-Tryptophan, N-acetyl-2,4,6-tribromo-1-[(1,1-dimethylethoxy)carbonyl]-5-methoxy-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



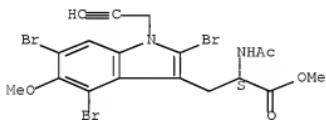
RN 920516-21-8 HCAPLUS  
 CN L-Tryptophan, N-acetyl-2,4,6-tribromo-5-methoxy-1-(2-propen-1-yl)-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



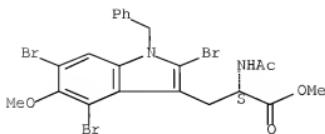
RN 920516-22-9 HCAPLUS  
 CN L-Tryptophan, N-acetyl-2,4,6-tribromo-5-methoxy-1-(2-propyn-1-yl)-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 920516-23-0 HCAPLUS  
 CN L-Tryptophan, N-acetyl-2,4,6-tribromo-5-methoxy-1-(phenylmethyl)-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 920516-24-1P

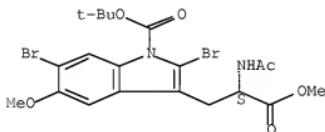
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(tryptophan derivs. for osteoporosis therapy)

RN 920516-24-1 HCAPLUS

CN L-Tryptophan, N-acetyl-2,6-dibromo-1-[(1,1-dimethylethoxy)carbonyl]-5-methoxy-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT.

L35 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2011 ACS on STN  
ACCESSION NUMBER: 2008:1237889 HCAPLUS Full-text

ACCESSION NUMBER: 2009.050.0001  
DOCUMENT NUMBER: 149:417852

TITLE: Novel bromo-melatonin derivatives as potentially effective drugs to treat bone diseases

AUTHOR(S): Suzuki, Nobuo; Somei, Masanori; Seki, Azusa; Reiter, Bussel J.; Hattori, Atsuhiko

CORPORATE SOURCE: *National Marine Laboratory, Inst. Nota Marine Laboratory, Inst.*

NOTE Marine Laboratory, Institute of Nature and Environmental Technology, Kanazawa University, Houshu-cho, Ishikawa, Japan

SOURCE: *Journal of Pineal Research*  
CODEN: JPRSEG, ISSN: 0742-1

PUBLISHER: COLLECTIF, ISSN: 0742-5660  
DOCUMENT TYPE: Wiley-Blackwell  
Journal: General Review

DOCUMENT TYPE: Journal, General  
LANGUAGE: English

LANGUAGE: ENGLISH  
FB: Estimated STN: 14 Oct 2008

ED ENTERED SIN: 14 Oct 2008

AB A review. Several report

#### regulation of bone metabo

### osteoclasts and osteoblasts

that contain osteoclasts, osteoblasts, and bone matrix, all of which are similar to those found in mammalian membrane bone. Using the assay, we demonstrated that melatonin suppressed osteoclastic and osteoblastic activities. These findings are in agreement with the reports from *in vivo* studies in mice and rats. In an attempt to develop mols. that increase bone

mass, novel bromo-melatonin derivs. were synthesized, and the effects of these chems. on osteoclasts and osteoblasts using the scale assay were examined. As a result, novel bromo-melatonin derivs. with the ability to possibly increase bone formation were identified. In scale osteoclasts, particularly, 1-benzyl-2,4,6-tribromo-melatonin had a more potent activity than melatonin. In reference to osteoblasts, this agent (10<sup>-9</sup>-10<sup>-6</sup> M) significantly activated osteoblasts. The effect of 1-benzyl-2,4,6-tribromo-melatonin on bone formation was confirmed in ovariectomized rats. Thus, the oral administration of 1-benzyl-2,4,6-tribromo-melatonin augmented the total bone mineral d. of the femoral metaphysis of ovariectomized rats. The stress-strain index of the diaphysis in 1-benzyl-2,4,6-tribromo-melatonin-treated rats significantly increased in comparison with that in ovariectomized rats. In rats fed a low-calcium diet, the total bone mineral d. of the femoral metaphysis significantly increased following the oral administration of 1-benzyl-2,4,6-tribromo-melatonin. These studies identified a melatonin derivative that may have potential use in the treatment of bone diseases, such as osteoporosis.

IT 864546-07-6, 1-Propargyl-2,4,6-Tribromo-melatonin

864546-08-7, 1-Allyl-2,4,6-Tribromo-melatonin

864546-09-8, 1-Benzyl-2,4,6-Tribromo-melatonin

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); TRU (Therapeutic use); BIOL (Biological study);

USES (Uses)

(novel bromo-melatonin derivs. as potentially effective drugs to treat bone diseases)

IT 864546-07-6, 1-Propargyl-2,4,6-Tribromo-melatonin

864546-08-7, 1-Allyl-2,4,6-Tribromo-melatonin

864546-09-8, 1-Benzyl-2,4,6-Tribromo-melatonin

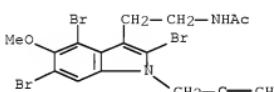
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); TRU (Therapeutic use); BIOL (Biological study);

USES (Uses)

(novel bromo-melatonin derivs. as potentially effective drugs to treat bone diseases)

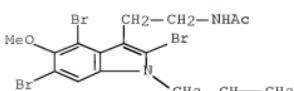
RN 864546-07-6 HCPLUS

CN Acetamide, N-[2-[2,4,6-tribromo-5-methoxy-1-(2-propyn-1-yl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)

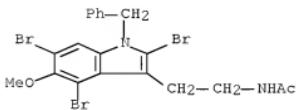


RN 864546-08-7 HCPLUS

CN Acetamide, N-[2-[2,4,6-tribromo-5-methoxy-1-(2-propen-1-yl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



RN 864546-09-8 HCPLUS  
 CN Acetamide, N-[2-[2,4,6-tribromo-5-methoxy-1-(phenylmethyl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS RECORD (12 CITINGS)  
 REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 3 OF 7 HCPLUS COPYRIGHT 2011 ACS on STN  
 ACCESSION NUMBER: 2008:462432 HCPLUS Full-text  
 DOCUMENT NUMBER: 149:45397  
 TITLE: Novel bromomelatonin derivatives suppress osteoclastic activity and increase osteoblastic activity: implications for the treatment of bone diseases  
 Suzuki, Nobuo; Somei, Masanori; Kitamura, Kei-Ichiro;  
 Reiter, Russel J.; Hattori, Atsuhiko  
 CORPORATE SOURCE: Noto Marine Laboratory, Institute of Nature and Environmental Technology, Kanazawa University,  
 Housu-gun, Ishikawa, Japan  
 SOURCE: Journal of Pineal Research (2008), 44(3), 326-334  
 CODEN: JPRSE9; ISSN: 0742-3098  
 PUBLISHER: Blackwell Publishing Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 15 Apr 2008  
 AB The teleost scale is a calcified tissue that contains osteoclasts, osteoblasts, and bone matrix, all of which are similar to those found in mammalian membrane bone. Using the goldfish scale, we recently developed a new *in vitro* assay system and previously demonstrated that melatonin suppressed both osteoclastic and osteoblastic activities in this assay system. In mammals, 2-bromomelatonin possesses a higher affinity for the melatonin receptor than does melatonin. Using a newly developed synthetic method, we synthesized 2-bromomelatonin, 2,4,6-tribromomelatonin and novel bromomelatonin derivs. (1-allyl-2,4,6-tribromomelatonin, 1-propargyl-2,4,6-tribromomelatonin, 1-benzyl-2,4,6-tribromomelatonin, and 2,4,6,7-tetrabromomelatonin) and then examined the effects of these chems. on osteoclasts and osteoblasts. All bromomelatonin derivs., as well as melatonin, had an inhibitory action on osteoclasts. In particular, 1-benzyl-2,4,6-tribromomelatonin (benzyl-tribromomelatonin) possessed a stronger activity than melatonin. At an *in vitro* concentration of 10-10 M, benzyl-tribromomelatonin still suppressed osteoclastic activity after 6 h of incubation. In reference to osteoblasts, all bromomelatonin derivs. had a stimulatory action, although melatonin inhibited osteoblastic activity. In addition, estrogen receptor mRNA expression (an osteoblastic marker) was increased in benzyl-tribromomelatonin (10-7 M)-treated scales. Taken together, the present results strongly suggest

that these novel melatonin derivs. have significant potential for use as beneficial drug for bone diseases such as osteoporosis.

IT 864546-07-6P, 1-Propargyl-2,4,6-tribromomelatonin

864546-08-7P, 1-Allyl-2,4,6-tribromomelatonin

864546-09-3P, 1-Benzyl-2,4,6-tribromomelatonin

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(novel bromomelatonin derivs. suppress osteoclastic activity and increase osteoblastic activity: implications for treatment of bone diseases)

IT 864546-07-6P, 1-Propargyl-2,4,6-tribromomelatonin

864546-08-7P, 1-Allyl-2,4,6-tribromomelatonin

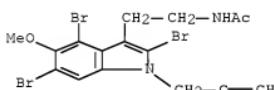
864546-09-3P, 1-Benzyl-2,4,6-tribromomelatonin

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(novel bromomelatonin derivs. suppress osteoclastic activity and increase osteoblastic activity: implications for treatment of bone diseases)

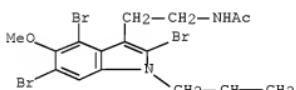
RN 864546-07-6 HCAPLUS

CN Acetamide, N-[2-[2,4,6-tribromo-5-methoxy-1-(2-propyn-1-yl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



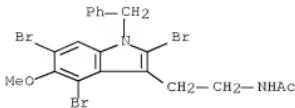
RN 864546-08-7 HCAPLUS

CN Acetamide, N-[2-[2,4,6-tribromo-5-methoxy-1-(2-propen-1-yl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



RN 864546-09-8 HCAPLUS

CN Acetamide, N-[2-[2,4,6-tribromo-5-methoxy-1-(phenylmethyl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD  
 (8 CITINGS)  
 REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

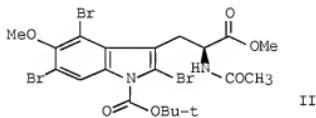
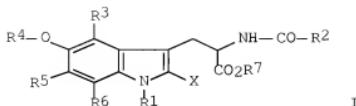
L35 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2011 ACS on STN  
 ACCESSION NUMBER: 2007:82570 HCAPLUS Full-text  
 DOCUMENT NUMBER: 146:163392  
 TITLE: Preparation of tryptophan derivatives for the treatment of osteoporosis  
 INVENTOR(S): Somei, Masanori; Hattori, Atsuhiko; Suzuki, Nobuo  
 PATENT ASSIGNEE(S): National University Corporation Kanazawa University, Japan; National University Corporation Tokyo Medical and Dental University  
 SOURCE: PCT Int. Appl., 28pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007010723	A1	20070125	WO 2006-JP312978	20060629 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1911744	A1	20080416	EP 2006-767595	20060629 <--
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CN 101233105	A	20080730	CN 2006-80026616	20060629 <--
CN 101233105	B	20101124		
US 7659304	B2	20100209	US 2008-7992	20080117 <--
US 20090054511	A1	20090226		
PRIORITY APPLN. INFO.:			JP 2005-209753	A 20050720 <--
			WO 2006-JP312978	W 20060629 <--

OTHER SOURCE(S): MARPAT 146:163392

ED Entered STN: 25 Jan 2007

GI



**AB** Title compds. I [X = halo; R1 = H, (un)substituted alkyl, (un)substituted alkenyl, etc.; R2 = (un)substituted alkyl; R3, R5, R6 = H, halo; R4 = H, (un)substituted alkyl; R7 = H, (un)substituted hydrocarbon group] and salts thereof were prepared. For example, reaction of (S)-N-acetyl-2,4,6-tribromo-5-methoxytryptophan Me ester, e.g., prepared from (S)-N-acetyl-5-methoxytryptophan Me ester, with BOC2O afforded compound II. The disclosed tryptophan derivs. were tested for the influences by tartarate resistant acid phosphatase (TRAP) and alkali phosphatase (ALP), and showed inhibition of osteoclast and activation of osteoblast.

IT 920516-24-1P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of tryptophan derivs. for the treatment of osteoporosis)

IT 920516-20-7P 920516-21-8P 920516-22-9P

920516-23-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of tryptophan derivs. for the treatment of osteoporosis)

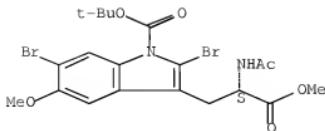
IT 920516-24-1P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of tryptophan derivs. for the treatment of osteoporosis)

RN 920516-24-1 HCPLUS

CN L-Tryptophan, N-acetyl-2,6-dibromo-1-[(1,1-dimethylethoxy)carbonyl]-5-methoxy-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 920516-20-7P 920516-21-8P 920516-22-9P

920516-23-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation);

THU (Therapeutic use); BIOL (Biological study); PREP

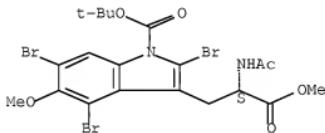
(Preparation); USES (Uses)

(preparation of tryptophan derivs. for the treatment of osteoporosis)

RN 920516-20-7 HCPLUS

CN L-Tryptophan, N-acetyl-2,4,6-tribromo-1-[(1,1-dimethylethoxy)carbonyl]-5-methoxy-, methyl ester (CA INDEX NAME)

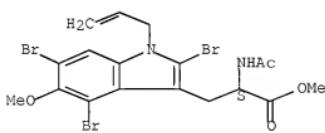
Absolute stereochemistry. Rotation (+).



RN 920516-21-8 HCPLUS

CN L-Tryptophan, N-acetyl-2,4,6-tribromo-5-methoxy-1-(2-propenyl)-, methyl ester (CA INDEX NAME)

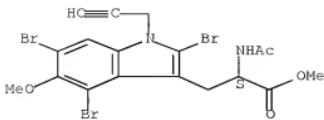
Absolute stereochemistry. Rotation (+).



RN 920516-22-9 HCPLUS

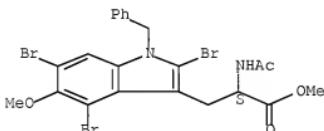
CN L-Tryptophan, N-acetyl-2,4,6-tribromo-5-methoxy-1-(2-propynyl)-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 920516-23-0 HCPLUS  
 CN L-Tryptophan, N-acetyl-2,4,6-tribromo-5-methoxy-1-(phenylmethyl)-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
 (1 CITINGS)  
 REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 5 OF 7 HCPLUS COPYRIGHT 2011 ACS on STN  
 ACCESSION NUMBER: 2006:1319103 HCPLUS [Full-text](#)  
 DOCUMENT NUMBER: 144:343589  
 TITLE: α2 RECEPTOR BLOCKING AGENT CONTAINING INDOLE  
 DERIVATIVE AS ACTIVE INGREDIENT AND VASODILATOR  
 INVENTOR(S): Somei, Masanori; Shigenobu, Koki; Tanaka, Yoshio  
 PATENT ASSIGNEE(S): National University Corporation Kanazawa University,  
 Japan; The Toho University  
 SOURCE: PCT Int. Appl., 22 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006035617	A1	20060406	WO 2005-JP17109	20050916 <-
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SI, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,				

CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,  
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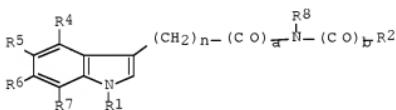
JP 2006089443	A 20060406	JP 2004-280104	20040927 <--
JP 3964417	B2 20070822		
US 20090005430	A1 20090101	US 2007-663748	20070823 <--
US 7872040	B2 20110118		

PRIORITY APPLN. INFO.:	MARPAT 144:343589	JP 2004-280104	A 20040927 <--
ED Entered STN:	06 Apr 2006	WO 2005-JP17109	W 20050916 <--

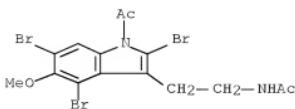
OTHER SOURCE(S):

ED Entered STN:

GI



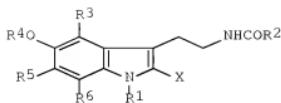
- AB A compound having a simpler structure than yohimbine, which is a pentacyclic fused heterocyclic compound, and having an activity similar to that of yohimbine. Also provided is an  $\alpha_2$  receptor blocking medicine or food composition containing either a compound represented by the formula : [Chemical formula I] (wherein R1 represents hydrogen, alkyl, alkenyl, alkynyl, an aromatic group, aralkyl, acyl, arylsulfonyl, alkylsulfonyl, or hydroxy; R2 represents a hydrocarbon group; R3, R4, R5, R6, and R7 are the same or different and each represents hydrogen, halogeno, alkyl, or alkoxy; R8 represents hydrogen or acyl; n is an integer of 1-6; and a and b are the same or different and each is 1 or 0) or a pharmaceutically acceptable salt thereof.
- IT 300662-22-0, 1-Acetyl-2,4,6-tribromomelatonin  
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (indole and melatonin derivs. as  $\alpha_2$ -adrenergic receptor antagonists and vasodilators)
- IT 300662-22-0, 1-Acetyl-2,4,6-tribromomelatonin  
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (indole and melatonin derivs. as  $\alpha_2$ -adrenergic receptor antagonists and vasodilators)
- RN 300662-22-0 HCPLUS
- CN Acetamide, N-[2-(1-acetyl-2,4,6-tribromo-5-methoxy-1H-indol-3-yl)ethyl]-  
 (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD  
 (2 CITINGS)  
 REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2011 ACS on STN  
 ACCESSION NUMBER: 2005:1004558 HCAPLUS Full-text  
 DOCUMENT NUMBER: 143:306168  
 TITLE: Preparation of indole derivatives for treatment of  
 osteoporosis  
 INVENTOR(S): Somei, Masanori; Hattori, Atsuhiko; Suzuki, Nobuo  
 PATENT ASSIGNEE(S): Kanazawa University Technology Licensing Organization  
 Ltd., Japan  
 SOURCE: PCT Int. Appl., 44 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005084664	A1	20050915	WO 2005-JP3743	20050304 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2005289985	A	20051020	JP 2005-61080	20050304 <--
JP 4014052	B2	20071128		
US 20070197629	A1	20070823	US 2006-591899	20060907 <--
PRIORITY APPLN. INFO.:			JP 2004-64408	A 20040308 <--
OTHER SOURCE(S): MARPAT 143:306168			WO 2005-JP3743	W 20050304 <--
ED Entered STN: 16 Sep 2005				
GI				



AB Title compds. represented by the formula I [wherein X = halo; R1 = H, (un)substituted alkyl, alkenyl, alkynyl, etc.; R2 = (un)substituted alkyl; R3, R5, R6 = independently H or halo; R4 = H or (un)substituted alkyl; and pharmaceutically acceptable salts thereof] were prepared for treatment of osteoporosis. For example, reaction of I (X = R3 = R5 = Br, R2 = R4 = Me, R1 = H) with propargyl chloride gave I (R2-R6 are defined as above, R1 = CH<sub>2</sub>-C≡CH) in 97% yield. The indole derivs. were tested for the influences received by bone cell (TRAP activity) and osteoblastic cell (ALP activity), and showed inhibition of osteoclast and activation of osteoblastic cell. Thus, I and their pharmaceutical compns. are useful for the treatment of osteoporosis.

IT 864546-07-6P 864546-08-7P 864546-09-8P

864546-10-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of indole derivs. for treatment of osteoporosis)

IT 864546-07-6P 864546-08-7P 864546-09-8P

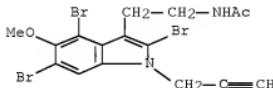
864546-10-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of indole derivs. for treatment of osteoporosis)

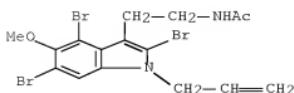
RN 864546-07-6 HCPLUS

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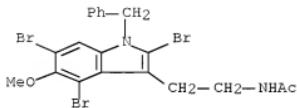


RN 864546-08-7 HCPLUS

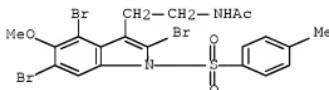
CN Acetamide, N-[2-[2,4,6-tribromo-5-methoxy-1-(2-propen-1-yl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



RN 864546-09-8 HCPLUS  
 CN Acetamide, N-[2-[2,4,6-tribromo-5-methoxy-1-(phenylmethyl)-1H-indol-3-yl]ethyl]- (CA INDEX NAME)

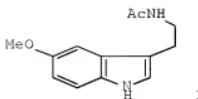


RN 864546-10-1 HCPLUS  
 CN Acetamide, N-[2-[2,4,6-tribromo-5-methoxy-1-[(4-methylphenyl)sulfonyl]-1H-indol-3-yl]ethyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD  
 (6 CITINGS)  
 REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 7 OF 7 HCPLUS COPYRIGHT 2011 ACS on STN  
 ACCESSION NUMBER: 2000:557901 HCPLUS [Full-text](#)  
 DOCUMENT NUMBER: 133:296316  
 TITLE: Syntheses of melatonin and its derivatives  
 AUTHOR(S): Somei, Masanori; Fukui, Yoshikazu; Hasegawa, Masakazu;  
 Oshikiri, Naoki; Hayashi, Toshikatsu  
 CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Kanazawa  
 University, Kanazawa, 920-0934, Japan  
 SOURCE: Heterocycles (2000), 53(8), 1725-1736  
 CODEN: HTCYAM; ISSN: 0385-5414  
 PUBLISHER: Japan Institute of Heterocyclic Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 133:296316  
 ED Entered STN: 14 Aug 2000  
 GI



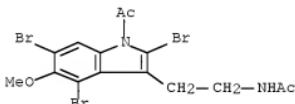
AB Two simple synthetic methods for melatonin (I) are newly developed from tryptamine through intermediates, which are promising lead compds. for drug developing research. Novel chemical reactivities of melatonin in its bromination, lithiation, and acylation are also reported.

IT 300662-22-0P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(synthesis of melatonin and derivs.)

IT 300662-22-0P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(synthesis of melatonin and derivs.)

RN 300662-22-0 HCPLUS

CN Acetamide, N-[2-(1-acetyl-2,4,6-tribromo-5-methoxy-1H-indol-3-yl)ethyl]-  
(CA INDEX NAME)

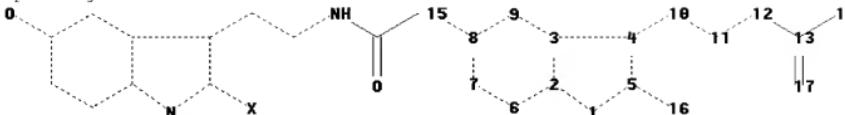


OS.CITING REF COUNT: 23 THERE ARE 23 CAPLUS RECORDS THAT CITE THIS  
RECORD (24 CITINGS)

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Structures uploaded into STN REGISTRY

Uploading L5.str



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10 11 12 13 14 15 16 17

ring nodes :  
1 2 3 4 5 6 7 8 9

chain bonds :  
4-10 5-16 8-15 10-11 11-12 12-13 13-14 13-17

ring bonds :  
1-2 1-5 2-3 2-6 3-4 3-9 4-5 6-7 7-8 8-9

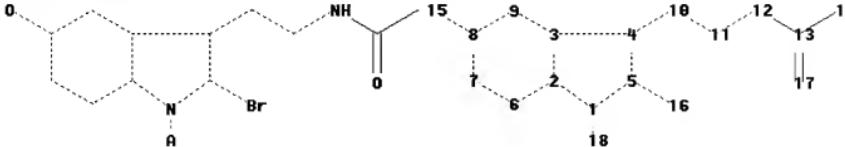
exact/norm bonds :  
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12-13 13-17

exact bonds :  
13-14

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS

Uploading L29.str



chain nodes :  
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ring nodes :  
1 2 3 4 5 6 7 8 9

ring/chain nodes :

18

chain bonds :  
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ring bonds :  
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exact/norm bonds :  
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11-12 12-13 13-17

exact bonds :  
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Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

Full search history

=> d his full

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FILE 'REGISTRY' ENTERED AT 15:38:13 ON 09 JUN 2011
L1      STRUCTURE uploaded
D L1
L2      0 SEA SSS SAM L1
L3      STRUCTURE uploaded
D L3
L4      0 SEA SSS SAM L3
L5      STRUCTURE uploaded
D L5
L6      1 SEA SSS SAM L5
D SCAN
L7      66 SEA SSS FUL L5
SAVE TEMP L7 PAG899STL5/A

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FILE 'REGISTRY' ENTERED AT 15:42:56 ON 09 JUN 2011

FILE 'REGISTRY' ENTERED AT 15:43:41 ON 09 JUN 2011
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D L9
L10     0 SEA SUB=L7 SSS SAM L9
L11     0 SEA SUB=L7 SSS FUL L9
L12     49 SEA SPE=ON ABB=ON PLU=ON L7 AND BR/ELS

FILE 'STNGUIDE' ENTERED AT 15:49:31 ON 09 JUN 2011

FILE 'REGISTRY' ENTERED AT 15:51:58 ON 09 JUN 2011
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D L13
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L15     0 SEA SUB=L7 SSS SAM L13

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L17     41 SEA SPE=ON ABB=ON PLU=ON L16 AND (AY<2007 OR PY<2007 OR
PRY<2007 OR REVIEW/DT)

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L19     20 SEA SPE=ON ABB=ON PLU=ON L7 AND 3/BR
L20     1 SEA SPE=ON ABB=ON PLU=ON L7 AND 4/BR
L21     0 SEA SPE=ON ABB=ON PLU=ON L7 AND 5/BR

FILE 'STNGUIDE' ENTERED AT 15:56:40 ON 09 JUN 2011

FILE 'REGISTRY' ENTERED AT 15:58:26 ON 09 JUN 2011
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D L22
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L24     7 SEA SUB=L7 SSS FUL L22
D SCAN
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10/591,899

L25            59 SEA SPE=ON ABB=ON PLU=ON L7 NOT L24  
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L28            0 SEA SUB=L7 SSS SAM L26  
L29            STRUCTURE uploaded  
               D L29  
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L31            18 SEA SUB=L7 SSS FUL L29  
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PRY<2007 OR REVIEW/DT)  
L34            6 SEA SPE=ON ABB=ON PLU=ON L32 AND (THU/RL OR DGN/RL OR  
DMA/RL OR PAC/RL OR PKT/RL OR ADV/RL)  
L35            7 SEA SPE=ON ABB=ON PLU=ON (L33 OR L34)  
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FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 8 JUN 2011 HIGHEST RN 1307949-22-9  
DICTIONARY FILE UPDATES: 8 JUN 2011 HIGHEST RN 1307949-22-9

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TSCA INFORMATION NOW CURRENT THROUGH January 14, 2011.

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predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

FILE HCAPLUS

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FILE COVERS 1907 - 9 Jun 2011 VOL 154 ISS 24  
FILE LAST UPDATED: 8 Jun 2011 (20110608/ED)  
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2011  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2011

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the fourth quarter of 2010.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE STNGUIDE  
FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Jun 3, 2011 (20110603/UP).